

**SciDAC Institute:  
Combinatorial Scientific Computing and Petascale Simulations (CSCAPES)  
ER 25774  
Alex Pothen  
Old Dominion University  
Final Report 2008**

**Personnel**

Alex Pothen (PI), Assefaw Gebremedhin (Research Scientist), Florin Dobrian (Consultant), Mahantesh Halappanavar (PhD student), Brandon Hill (Master's student), Min Huang (PhD student), Duc Nguyen (Undergraduate student)

**Research**

We have made progress on a number of research areas in combinatorial scientific computing.

In Automatic Differentiation (AD), we developed the first practical algorithm for acyclic coloring, and a faster algorithm for computing star coloring; both of these are specialized graph coloring algorithms that arise in the context of computing large, sparse Hessian (second derivative) matrices. These algorithms were implemented, and the software was used incorporated into an AD tool called ADOL-C. Our coloring software for computing Jacobians and Hessians, and ADOL-C were used to solve optimization problems from two applications: controlling an electrical power grid, and designing a simulated moving bed (SMB) chromatographic purification process in chemical engineering. We also improved the algorithm for detecting sparsity in ADOL-C by several orders of magnitude. In the SMB case, we computed Jacobian matrices with millions of rows and columns in about a hundred times the time needed to compute the function to be optimized. We are continuing to work with chemical engineers from Georgia Tech on the SMB design.

We have also developed parallel coloring algorithms for the distance-2 coloring problem, which is used for computing Jacobian (first derivative) matrices. Techniques such as graph partitioning, speculative coloring to enhance the concurrency in the computation, detection of incorrectly colored vertices, and resolving such conflicts, were used to obtain speed-ups for the coloring algorithm for up to a hundred processors. We are currently working on extending this work to larger numbers of processors to scale up to tera- and peta-scale machines.

We have developed the first  $2/3$ -approximation algorithm for the vertex weighted matching problem. The matching problem has applications in the load balancing work that will be done as part of the CSCAPES Institute, and to large sparse matrix computations. We developed the first parallel algorithm for computing an approximate matching for the edge-weighted matching problem on thousands of processors, extending recent work by Hoepman and Manne. Matching has applications to many areas of computer science and CSE, but is also a prototype of a combinatorial problem which is challenging to parallelize on petascale architectures. This is our reason for working on parallel matching.

### **Software**

Our parallel coloring software has been integrated with the Zoltan software library, being developed by our colleagues Sandia National Labs as part of the CSCAPES Institute. Our software package for coloring, COLPACK, has been integrated with a software library for Automatic Differentiation called ADOL-C, and has also been released for use on the CSCAPES web site ([www.cscapes.org](http://www.cscapes.org)). Our software for exact and approximate matchings, being developed in MatchBox and MatchBoxP, are being used by the Sandia team in the CSCAPES project.

### **Outreach**

Alex Pothén served on the George Polya prize committee, the nomination committee for the SIAM CSE Activity Group, and on the organizing committee for the SIAM Conference on CSE to be held in March 2009 in Miami, FL. We organized an CSCAPES Workshop in June in Santa Fe NM, which was attended by participants in several SciDAC projects as well as all CSCAPES researchers. We presented a poster and contributed a paper at the 2008 SciDAC conference.

The following talks were given.

1. *Automatic Differentiation and Combinatorics: An accidental partnership?* Automatic Differentiation 2008, Bonn, Germany, August 2008.
2. *Exploiting sparsity in Jacobian computation via coloring and AD: A case study in a simulated moving bed process*, Automatic Differentiation 2008, Bonn, Germany, August 2008.
3. *CSCAPES Institute: Recent Progress*, Poster, SciDAC 2008 Conference, Seattle, July 2008.
4. *Approximation Algorithms for vertex weighted matching*, SIAM Conference on Discrete Mathematics, Burlington VT June 2008.

5. *CSCAPES Workshop*, Ten talks, Santa Fe NM, June 2008.
6. *New acyclic and star coloring algorithms and application to Automatic Differentiation*, SIAM Conference on Optimization, Boston May 2008.
7. *A scalable algorithmic framework for parallel graph coloring on distributed memory computers*, SIAM Conference on Parallel Computing, Atlanta, March 2008.
8. *Combinatorial Algorithms Enabling Peta-scale Computational Science*, SciDAC Conference, Department of Energy, Boston, June 2007 (Invited Talk)
9. *The CSCAPES Institute: Vision and Plans*, SIAM Conference on Computational Science, Costa Mesa CA, 2007.
10. *Graph Coloring Algorithms for Efficient Automatic Differentiation*, SIAM Workshop on Combinatorial Scientific Computing, Costa Mesa CA, 2007.
11. *Computing Derivatives without Tears: Graph Coloring and Automatic Differentiation*, ICIAM, Zurich, July 2007.
12. *Approximation Algorithms for Vertex Weighted Matching*, ICIAM, Zurich, July 2007.

### **CSCAPES Institute Web Page**

Alex Pothén serves as the PI of the CSCAPES Institute. The URL [www.cscapes.org](http://www.cscapes.org) provides more information on the activities of the Institute personnel.

### **Recruiting**

Assefaw Gebremedhin has joined Purdue University as a Research Assistant Professor, and will continue with the CSCAPES Institute, centered at Purdue (since the PI Alex Pothén has moved to Purdue). Florin Dobrian has joined the Conviva Corporation, but continues to work with us as a consultant. Dun Nguyen will complete his undergraduate degree in Fall 2008, and is applying to graduate schools, including Purdue. Min Huang has begun coursework at Purdue with a view to obtaining a PhD degree.

### **References**

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4. Erik G. Boman, Doruk Bozdag, Alex Pothén et al., Enabling high performance computational science through combinatorial algorithms, *Journal of Physics: Conference Series* 78 (012058), 10 pp., 2007.
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10. Florin Dobrian, Mahantesh Halappanavar, and Alex Pothén, A 2/3-approximation algorithm for vertex weighted matching, submitted to *ACM Transactions on Algorithms*, 2008.